Connection between the "Strutinsky level density" and the semiclassical level density

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We establish an analytical link between the level density obtained by means of the Strutinsky averaging method, and the semiclassical level density. This link occurs only in the so-called "asymptotic limit".

It turns out that the Strutinsky method amounts to an approximation to the semiclassical method. This approximation contains an unavoidable remainder which constitutes an intrinsic noise in comparison to the semiclassical method. Thus, the "old" problem of the dependency of the Strutinsky procedure on the two free smoothing parameters of the averaging is intimately connected to this noise.

On the other hand, we demonstrate that the noise of the method is small in the average density of states and in the average energy, whereas it might be non-negligible in the shell correction itself. In order to improve this method, we give a "rule" which consists simply of minimizing the relative error made on the average energy.

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I. INTRODUCTION

The inclusion of the Strutinsky's shell correction [1]-[3] in the liquid- drop model [4], namely the so-called macroscopic-microscopic method, has allowed considerable improvements in the predictions of the nuclear masses [5], and in the calculations of the fission barriers, as well [7],[9]. Nowadays, despite the progress of the more basic microscopic models (such as self-consistent models), it remains often used.

This method consists essentially of combining the liquid-drop model (macroscopic model) where the binding energy varies slowly as a function of the number of nucleons N and Z, with a shell correction varying abruptly with N and Z. The latter is due to the non-uniformity of the shell structure of the energy levels. It is extracted from a single-particle Hamiltonian (microscopic model) according to an original idea of Strutinsky.

The Strutinsky method is mainly based on a particular smoothing procedure of the density of states.

Although this method is very efficient, it contains two weak points which are:

1) The dependence of the results on the two well known inherent parameters, i.e. the width γ and the order M of the smoothing

2) The difficulties of the treatment of the continuum encountered with realistic mean potentials

The purpose of the present work is summarized in the following points:

1) The Strutinsky method can be derived rigorously from the point of view of the least-squares approximation of the level density. The equivalence between this point of view and the well-known standard averaging appears trivial.

2) In this work, it is proved analytically that the averaged level density obtained by the Strutinsky method is simply an approximation to the semiclassical level density.
In this respect, the semiclassical level density can be considered as the "true" (i.e. exact) smooth density.

3) It is mainly shown that in comparison with the semiclassical method, the Strutinsky method is characterized by a remainder which contains all the dependence on the two smoothing (free) parameters, and which is thence, the source of the "noise" of the averaging procedure.

4) Concerning the smooth density of states and the smooth energy, it is demonstrated that the Strutinsky method is reliable. However, the shell correction itself must be treated with care because it is very sensitive to the choice of the two free averaging parameters. In this context, in order to improve the method, we propose the "rule of the relative remainder" (RRR rule).

5) At last, it is explained why the Strutinsky method fails near the zero-energy (top of the well) for finite mean potentials

II. THE STRUTINSKY AVERAGING

A. Bases and phenomenology of the Strutinsky's method

In spite of the complexity of the nuclear forces, it appears that most of the binding energy of the nuclei is well described by the so-called liquid-drop model. This

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simple phenomenological approach is of a classical type. This means that the quantum effects, or a more precisely, the shell effects, are ignored by this model. This causes systematic discrepancies between the theoretical predictions and the experimental data
On the other hand, it is known that such effects are contained in the shell model, but the latter is unable to reproduce correctly the general trends of the binding energy. To solve this dilemma, Strutinsky has proposed to combine the binding energy of the liquid-drop model with a small (but essential) correction deduced from the shell model. This can be written as:

$$\begin{aligned} E \text{ (Binding Energy)} &= E \text{ (Liquid Drop Model)} \\ &\quad +\delta E \text{ (Shell Correction)} \end{aligned}$$

The shell correction is calculated from a mathematical prescription outlined by Strutinsky

It is obtained by summing the single particle energies of a phenomenological shell model potential and subtracting the average (smooth) part of this quantity:

$$\delta E \text{ (Shell Correction)} = \sum_i \epsilon_i - \overline{\sum_i \epsilon_i}$$

As already mentioned, this method is often called the macroscopic-microscopic method because it mixes two very different models. Such a duality is obviously not free from inconsistency. Nevertheless, it is possible to give a microscopic basis to this "model" within the Hartree-Fock (HF) approximation and some simple assumptions [2],[3].
This consists essentially of expanding the HF energy around its semiclassical approximation obtaining thus the so-called "Strutinsky energy theorem":

$$E(\rho) = E(\overline{\rho}) + \left(\sum_i \epsilon_i - \overline{\sum_i \epsilon_i} \right) + O_2 \qquad (1)$$

Here ρ is the HF density matrix, and $\overline{\rho}$ its semiclassical approximation which is a smooth quantity, free of shell effects. For this reason $\overline{\rho}$ can be assimilated to the classical average (i.e. without quantal variations) part of ρ. The sums of single-particle energies $\Sigma\epsilon_i$ and $\overline{\Sigma\epsilon_i}$ are related respectively to ρ and $\overline{\rho}$. Finally, O_2 is a quantity of the second order in the operator $\rho - \overline{\rho}$, and is generally negligible (for details see [28]).

It is clear from (1) that the macroscopic-microscopic method described above is a "schematic" interpretation of this theorem. The quantity $E(\overline{\rho})$ can be replaced by the energy of the liquid-drop formula, and the shell correction is deduced from a phenomenological one body Hamiltonian
It is also to be noted that a complete microscopic approach of this theorem remains possible. For example, in ref. [27] the authors use a method referred to as the Extended Thomas Fermi plus Strutinsky integral (ETFSI) method. In the latter, the semiclassical quantity $E(\overline{\rho})$ is deduced self-consistently from a microscopic effective interaction.(Skyrme III). The shell correction is then added to $E(\overline{\rho})$.

In the following, we will mainly focus on two points:

- The mathematical aspect of the Strutinsky smoothing
- The link between this smoothing and the semiclassical approximation, and its consequences

B. The "exact" level density

The Strutinsky averaging can be derived by various formal approaches [1]-[3], [7], [9]-[11].
In this work, we will derive it from the point of view of the least-squares approximation. In fact, this point has been early suggested by Bunatian and co-authors [19]. The least-squares approximation will help us to understand why the Strutinsky averaging fails near the edge of realistic potentials.
For an entirely discrete spectrum the level density of states is defined by:

$$g_o(\epsilon) = \sum_{n=0}^{\infty} \delta(\epsilon - \epsilon_n) \qquad (2)$$

In the following, this density will be called the "exact quantum level density", or shortly, the "exact level density", because it is a true quantum quantity, as opposed to its semiclassical approximation, or as opposed to the level density obtained from $g_o(\epsilon)$ by the Strutinsky averaging (see below).

In fact, Eq.(2) concerns uniquely infinite potentials without continuum. Finite potentials will be treated separately at the end of this paper.

C. Polynomial approximation to the "exact" level density:

Let $g_M(\epsilon)$ be a polynomial approximation of order M to the "exact" level density. More precisely, we seek this approximation in the vicinity of a point λ (which represents actually the Fermi level) in an effective interval $[-\gamma + \lambda, \lambda + \gamma]$, by using the Gaussian weight $\exp\left(-(\epsilon - \lambda)^2/\gamma^2\right)$. For this reason, the cited polynomial must depend a priori not only on M, but also on γ and λ. Therefore, it will be denoted $\overline{g}_{M\ ,\gamma}(\epsilon, \lambda)$. For our purpose, it will be convenient to write this polynomial as a linear combination of Hermite polynomials H_k.

$$\overline{g}_{M\ ,\gamma}(\epsilon, \lambda) = \sum_{k=0}^{M} c_k H_k \left(\frac{\epsilon - \lambda}{\gamma} \right)$$

Thus, We must look for the polynomial $g_{M\ ,\gamma}(\epsilon,\lambda)$ which minimizes the integral:

$$I(\lambda,M,\gamma)=\int_{-\infty}^{\infty}\left[g_o(\epsilon)-\overline{g}_{M\ ,\gamma}(\epsilon,\lambda)\right]^2 e^{-\left(\frac{\epsilon-\lambda}{\gamma}\right)^2}d\epsilon \tag{3}$$

This procedure is a local averaging in the sense of the least- squares fit. Minimizing (3) with respect to the coefficients c_k , and using the orthogonality property of the Hermite polynomials we find:

$$\overline{g}_{M\ ,\gamma}(\epsilon,\lambda)=\sum_{m=0}^{M}c_m(\lambda,\gamma)H_m(\frac{\epsilon-\lambda}{\gamma}) \tag{4}$$

$$c_m(\lambda,\gamma)=\frac{1}{m!2^m\sqrt{\pi}}\sum_{n=0}^{\infty}H_m(u_n)\frac{1}{\gamma}\exp\left[-u_n^2\right],$$

$$u_n=\frac{\epsilon_n-\lambda}{\gamma}$$

As we shall see in the next subsection, Eq.(4) is not the final definition of the averaging which thus appears somewhat more "subtle".

D. The Strutinsky's averaging as a moving average

In Eq.(4) the Fermi level λ is supposed to be fixed, and the polynomial $\overline{g}_{M\ ,\gamma}(\epsilon,\lambda)$ smoothes the exact level density only in the vicinity of λ. Thus only a part of the spectrum is " smoothed", i.e. the part $\epsilon\simeq\lambda$. To avoid this drawback, it is necessary to consider λ as a variable. The averaged level density is thus defined as $\overline{g}_{M\ ,\gamma}(\epsilon,\lambda)$ making $\epsilon=\lambda$. This amounts to perform a moving average (i.e. λ is moved with ϵ, "centering" ϵ on λ).
In the following, we shall call up the function $g_{_M,\gamma}(\lambda,\lambda)$ as the Strutinsky's level density, and we will note it simply by $\overline{g}_{_M,\gamma}(\lambda)$.
Since the coefficients c_m in (4) depend on λ, the Strutinsky's quantity $\overline{g}_{M\ ,\gamma}(\lambda)$ is, in general, not a polynomial in λ. However, it is clear that, although the Strutinsky level density is not really a polynomial, it behaves locally ($\sim\lambda\pm\gamma$), like a least deviating polynomial approximation for the exact level density $g_o(\lambda)$ given by (2).

Explicitly, we must replace ϵ with λ in (4):

$$\overline{g}_{M\ ,\gamma}(\lambda)=\sum_{n=0}^{\infty}F_M\left(u_n\right),\quad u_n=\frac{\epsilon_n-\lambda}{\gamma} \tag{5}$$

$$F_M\left(x\right)=\widetilde{P}_M\left(x\right)\frac{1}{\gamma}\exp\left(-\,x^2\right)$$

$$\widetilde{P}_M\left(x\right)=\sum_{m=0}^{M}A_mH_m\left(x\right),\quad A_m=\frac{H_m(0)}{m!2^m\sqrt{\pi}}$$

$$H_m(0)=(-1)^{m/2}.m!/\left(m/2\right)!\ \text{ if } m \text{ is even},$$

$$H_m(0)=0\ \text{ if } m \text{ is odd}$$

In (5) the polynomial $\widetilde{P_M}$ constitutes the so-called curvature correction term.

It is easy to check that the expression (5) obtained from a least-squares fitting, can be written as the usual folding procedure of the exact level density [14],[18]:

$$\overline{g}_{_{M,\gamma}}(\lambda)=\int_{-\infty}^{\infty}g_o(\epsilon)F_M\left(\frac{\epsilon-\lambda}{\gamma}\right)d\epsilon \tag{6}$$

which demonstrates the equivalence between the two points of view, i.e. between the local least square smoothing (3) and the averaging (6).

Remark:
It is to be noted that if M increases to infinity and/or γ decreases to zero, then $\overline{g}_{_{M,\gamma}}$ tends toward $g_o(\epsilon)$. Obviously, in practice these parameters are finite.

E. Necessary condition in the smoothing procedure

The least-square smoothing (3) or its equivalent (6) gives an approximation *to the exact level density* (2). Therefore, if the averaging is too accurate (see the previous remark) the procedure leads to a curve which is very close to (2). This curve remains characterized by strong oscillations which express shell effects. However, the aim of the Strutinsky method is precisely to remove these shell effects.

For $M=0$, the effective interval of averaging is governed by a pure Gaussian (since $\widetilde{P}_0(x)=1$ in (5)). In order to wipe out the shell effects from the averaging , the parameter γ must be at least of the order of the mean spacing between the shells.(denoted here by $\overline{\hbar\omega}$) near the Fermi level:

$$\gamma\gtrsim\overline{\hbar\omega} \tag{7}$$

In this way, we obtain a "true" smooth density.

If Eq.(7) is not satisfied, the level density remains characterized by oscillations (quantum effects) and are in opposition with the character of the semiclassical density.

For $M>0$, F_M is not a pure Gaussian anymore, and, this case becomes more complicated. Indeed, the width of the averaging function F_M is not really γ, because in

(5) the Gaussian is modulated by the polynomial $\widetilde{P}_M$. It turns out that to maintain this width of the order of mean spacing shell we have to enlarge the parameter γ with respect to the order M. Thus, the smoothing procedure implies a "coherency" between these two parameters.

Usually, the couple (γ, M) is determined by the so-called plateau condition [18] from the typical ranges: $6 \lesssim M \lesssim 20$, and, $\overline{\hbar\omega} \lesssim \gamma \lesssim 2\overline{\hbar\omega}$.

Due to the above "coherency", it is easy to notice that the plateau is invariably moved towards the right-hand side (toward the largest γ), when M increases.

Since in the harmonic oscillator the spacing between the shells is constant, we have in this simple case $\overline{\hbar\omega} = \hbar\omega$.

Fig.1 displays the Strutinsky level density (calculated from Rel.(5)) for three values of the parameter γ.(M being fixed).

Curve(a): Since γ is too small compared to $\hbar\omega$ the curve (a) is characterized by strong oscillations (shell effects) which are close to Dirac functions (see Rel.(2)).
Curve (b): By increasing γ one diminishes the magnitude of these oscillations.
Curve (c): In the third case, γ is of the order of $\hbar\omega$, the curve becomes smooth, and can be regarded as the mean behavior of the exact level density (the so-called smooth component contained in the exact level density (2)).

F. Averaged particle-number, averaged energy, and shell correction

The averaged particle-number and the averaged energy are defined through the average density of states $\overline{g}_{M,\gamma}$ by:

$$\overline{N}_{M,\gamma}(\lambda) = \int_{-\infty}^{\lambda} \overline{g}_{M,\gamma}(\epsilon)d\epsilon \tag{8}$$

$$\overline{E}_{M,\gamma}(\lambda) = \int_{-\infty}^{\lambda} \epsilon\overline{g}_{M,\gamma}(\epsilon)d\epsilon \tag{9}$$

The detailed expressions are given in Ref.[9].

In practice the upper bound of the integral giving the particle-number is deduced from the equation

$$\overline{N}_{M,\gamma}(\lambda) = N_0 \tag{10}$$

where N_0 is the particle-number of the system. The quantity λ is the Fermi level of the average density $\overline{g}_{M,\gamma}$ (i.e. the Strutinsky level density)

Finally the Strutinsky shell correction to the binding energy of the liquid drop model is defined as follows :

$$\delta\overline{E}_{M,\gamma} = \int_{-\infty}^{\lambda_0} \epsilon g_o(\epsilon)d\epsilon - \int_{-\infty}^{\lambda} \epsilon\overline{g}_{M,\gamma}(\epsilon)d\epsilon = \sum_{n=0}^{N_0} \epsilon_n - \overline{E}_{M,\gamma}(\lambda) \tag{11}$$

Where $g_o(\epsilon)$ is the exact level density given by (2) and λ_0 is its Fermi level (the last occupied level). Sometimes, $\overline{E}_{M,\gamma}(\lambda)$ is denoted as $\overline{\sum \epsilon_n}$.

In Rel.(11), the shell correction should not contain any component of the smooth energy which is by definition already included in the liquid drop model. Consequently, the average density $\overline{g}_{M,\gamma}$ (or the average energy $\overline{E}_{M,\gamma}(\lambda)$) must not contain any residual shell effect.
Moreover, since $\overline{g}_{M,\gamma}$is a least square approximation of g_o, one can write $g_o \approx g_{M,\gamma} + \delta g_{M,\gamma}$, with $\lambda_0 \approx \lambda$. When the condition (7) is fulfilled, $g_{M,\gamma}$ becomes smooth and the exact density g_o oscillates around $g_{M,\gamma}$ making $\delta g_{M,\gamma}$ alternatively positive and negative. Consequently, from (11) one can deduce formally that:

$$\delta\overline{E}_{M,\gamma}(\lambda) \approx \int_{-\infty}^{\lambda} \epsilon\delta g_{M,\gamma}(\epsilon)d\epsilon \tag{12}$$

Thus, the oscillations of the shell correction $\delta\overline{E}_{M,\gamma}(\lambda)$ as a function of λ are due to the fluctuations of $\delta g_{M,\gamma}(\epsilon)$.

Note:
In practice, due to the finite size of the spectrum, for the shell correction, the following cut-off condition $\epsilon_{last\text{-}level} - \lambda \gg \gamma$ must be required (see [18])

III. THE SEMICLASSICAL LEVEL DENSITY

A. Bohr's correspondence principle

Although the Strutinsky level density is mathematically well defined by (5), there is no physical basis for this smoothing. Consequently, it is necessary to build an other level density free of shell effects which would be justified by physical arguments.

Shell effects are the consequence of the quantum nature of the level distribution (2). The natural way to eliminate such effects would be to go over to the classical limit. To this end, we will apply the correspondence principle (Bohr 1923) which states that the behavior of quantum systems reduces to classical physics in "the limit of large quantum numbers".
Starting from this principle, the semiclassical level density can be deduced by using the Euler-Maclaurin (EML) summation formula.
In practice, this amounts to obtain an asymptotic series which contains only three or four terms, all the others being divergent. The first term of this series coincides with the known Thomas-Fermi approximation.
The EML expansion used here is equivalent to the

usual standard semiclassical methods, e.g., the Wigner-Kirkwood expansion [13],[15],[16], or the method of the partition function [20]. The latter are based on asymptotic series of powers of $\hbar$. Indeed, in the correspondence principle, the limit of large quantum numbers amounts to taking the classical limit $\hbar \to 0$.

B. "Asymptotic limit of large quantum numbers"

In practical cases, the concept of "large quantum numbers" must be précised by a more concrete definition. To illustrate this point, we start from the typical example of the three-dimensional harmonic oscillator. Such system is very simple, its energy levels are given by:

$\epsilon_n = (n + 3/2)\hbar\omega, \qquad n = 0, 1, 2, 3, ..\infty$

The quantum number n defines a shell, and $\hbar\omega$ represents the gap between these shells.

Thus, n is given by:

$n = (\epsilon_n - \epsilon_0)/\hbar\omega$ here $\epsilon_0 = (3/2)\,\hbar\omega$ is the lowest level of the spectrum

The correspondence principle states that for large values of $n = (\epsilon_n - \epsilon_0)/\hbar\omega$, the quantum physics reduces to classical physics, in particular, the quantum (exact) level density $g_o(\lambda)$ defined by (2) should approach the semiclassical level density denoted here by $g_{sc}(\lambda)$. This can be written as :

if $n = [(\epsilon_n - \epsilon_0)/\hbar\omega] \to \infty$, then $g_o \to g_{sc}$

As already noted, the shell effects are mainly determined by the small part of the spectrum $\{\epsilon_n\}$ which is located in the vicinity of the Fermi level λ. Consequently for these levels, we have roughly $\epsilon_n \approx \lambda$, and, this limit becomes:

if $n = [(\lambda - \epsilon_0)/\hbar\omega] \to \infty$, then $g_o(\lambda) \to g_{sc}(\lambda)$

Since in general the Fermi level increases with the quantum numbers, the arguments presented for the harmonic oscillator are also valid for any other physical system. Therefore, we will consider the previous statement as general. However, we must now redefine $\hbar\omega$ as the mean shell-spacing in the neighborhood of the Fermi level λ. As in Rel.(7), we denote it by $\overline{\hbar\omega}$.

$$\text{if} \quad \frac{(\lambda - \epsilon_0)}{\overline{\hbar\omega}} \to \infty, \quad \text{then} \qquad g_o(\lambda) \to g_{sc}(\lambda) \quad (13)$$

This limit is of course unphysical. Therefore in practice, we require the following qualitative criterion:

$$\text{if} \quad \frac{\lambda - \epsilon_0}{\overline{\hbar\omega}} \gg 1 \qquad \text{then} \qquad g_o(\lambda) \approx g_{sc}(\lambda) \qquad (14)$$

We understand by (14) that $\left[(\lambda - \epsilon_0)/\overline{\hbar\omega}\right]$ is sufficiently large compared to the unity so that $g_o(\lambda)$ can be considered as close as possible to $g_{sc}(\lambda)$ with a "satisfactory accuracy".

Finally, the "asymptotic limit of large quantum numbers" can be defined theoretically by (13), or practically by (14).

Notes:

In practical cases, $\lambda \gg \epsilon_0$, therefore the previous requirement can be replaced with $\lambda/\overline{\hbar\omega} \gg 1$. In this case, the Fermi level λ must be measured from the bottom of the well

C. Two well-known analytical cases

The procedure described above is applied in appendix B to two simple cases.

1. *The semiclassical level density of the harmonic oscillator*

The eigenenergies of the isotropic oscillator are :

$$E_{n_x,n_y,n_z} = (n_x + n_y + n_z + \frac{3}{2})\hbar\omega_0 \qquad (15)$$
$$n_x, n_y, n_z = 0, 1, 2, ...\infty$$

The semiclassical level density of the harmonic oscillator is a simple parabola (see appendix B):

$$g_{sc.}(\lambda) = \frac{1}{2}\frac{\lambda^2}{(\hbar\omega_0)^3} - \frac{1}{8}\frac{1}{\hbar\omega_0} \qquad (16)$$

This result is well-known, and was established very early by means of the partition function [20], or more recently by the Wigner-Kirkwood expansion [21].

2. *The semiclassical level density of the infinitely deep cubic box*

For the case of cubic box with totally reflecting walls the spectrum is given by:

$$E_{n_x n_y n_z} = \left(n_x^2 + n_y^2 + n_z^2\right) E_0 \qquad (17)$$
$$E_0 = \pi^2\hbar^2/\left(2ma_0^2\right),\ a_0 = \text{side of the cubic box}$$
$$n_x, n_y, n_z = 1, 2, ...\infty$$

The semiclassical level density of the infinite cubic box (see appendix B) is also an "old " result [20], [22].

$$g_{sc.}(\lambda) \approx \frac{1}{E_0^{3/2}}\frac{\pi}{4}\sqrt{\lambda} - \frac{3\pi}{8}\frac{1}{E_0} + \frac{3}{8}\frac{1}{E_0^{1/2}}\frac{1}{\sqrt{\lambda}} \qquad (18)$$

D. Semiclassical shell correction

We define the semiclassical energy by a very similar relations to (8-11), replacing the Strutinsky level density

by the one of the semiclassical density. The corresponding Fermi level is denoted as λ_{sc}.

$$N_{sc}(\lambda_{sc}) = \int_{-\infty}^{\lambda_{sc}} g_{sc}(\epsilon)d\epsilon \tag{19}$$

$$E_{sc}(\lambda_{sc}) = \int_{-\infty}^{\lambda_{sc}} \epsilon g_{sc}(\epsilon)d\epsilon \tag{20}$$

$$N_{sc}(\lambda_{sc}) = N_0 \tag{21}$$

$$\delta E_{sc} = \int_{-\infty}^{\lambda_0} \epsilon g_o(\epsilon)d\epsilon - \int_{-\infty}^{\lambda_{sc}} \epsilon g_{sc}(\epsilon)d\epsilon = \sum_{n=0}^{N_0} \epsilon_n - E_{sc}(\lambda_{sc}) \tag{22}$$

One must note that unlike $\delta\overline{E}_{M,\gamma}(\lambda)$, the quantity δE_{sc} does not depend on any free parameter.

IV. THE CONNECTION BETWEEN THE "STRUTINSKY'S LEVEL DENSITY" AND THE SEMI-CLASSICAL LEVEL DENSITY.

A. Assumptions and quantitative approach of the asymptotic limit

We know from the Bohr principle given in subsect. III B that in the "asymptotic limit" (14) we must have the approximation $g_o(\lambda) \simeq g_{sc}(\lambda)$. Since the Strutinsky averaging (6) gives an approximation to the exact level density $g_o(\lambda)$, normally in this limit it should also give an approximation to the semiclassical level density $g_{sc}(\lambda)$. The role of the curvature correction term would be to improve the approximation.

We start from the averaging (6), substituting $g_{sc}(\lambda)$ for $g_o(\lambda)$ in the "asymptotic limit"(14). In the Strutinsky averaging the parameter γ must be of the order of the mean shell spacing $\overline{\hbar\omega}$ near the Fermi level (see Eq.(7)). Consequently, in Rel.(14) we should replace $\overline{\hbar\omega}$ with γ.

$$\overline{g}_{_{M,\gamma}}(\lambda) \approx \int_{-\infty}^{\infty} g_{sc}(\epsilon)\widetilde{P_M}\left(\frac{\epsilon-\lambda}{\gamma}\right)\frac{1}{\gamma}\exp\left(-\left(\frac{\epsilon-\lambda}{\gamma}\right)^2\right)d\epsilon \tag{23}$$

$$\text{with } \frac{\lambda-\epsilon_0}{\gamma} \gg 1, \quad \text{and } \gamma \gtrsim \overline{\hbar\omega} \tag{24}$$

Making $X = \dfrac{\epsilon-\lambda}{\gamma}$, we obtain:

$$\overline{g}_{_{M,\gamma}}(\lambda) \approx \int_{-\infty}^{\infty} g_{sc}(\lambda+\gamma X)\widetilde{P_M}(X)\exp\left(-X^2\right)dX, \quad M \text{ even}$$

Now, one replaces the semiclassical density $g_{sc}(\lambda+\gamma X)$ by its $(M+2)$ first terms of the Taylor expansion around λ (M must be even in $\widetilde{P}_M(X)$). The last term gives an estimation of the remainder:

$$\overline{g}_{_{M,\gamma}}(\lambda) \approx \int_{-\infty}^{\infty} [g_{sc}(\lambda) + \sum_{k=1}^{M+1}\frac{(\gamma X)^k}{k!}\frac{d^k g_{sc}(\lambda)}{d\lambda^k} + \frac{(\gamma X)^{M+2}}{(M+2)!}\frac{d^{M+2}g_{sc}(\lambda)}{d\lambda^{M+2}}]\widetilde{P}_M(X)\exp\left(-X^2\right)dX$$

It is easy to show that $\widetilde{P}_M(X)\exp\left(-X^2\right)$ behaves like a delta function with respect to any polynomial of order $k \leq M$. Consequently the first term gives back $g_{sc}(\lambda)$, and the second has no contribution (by noticing that X^{M+1} is odd). The remaining integral, i.e.:

$I(M) = \int_{-\infty}^{\infty} X^{M+2}\widetilde{P}_M(X)\exp\left(-X^2\right)dX$

is obtained from appendix A.

Finally:

$$\overline{g}_{_{M,\gamma}}(\lambda) \approx g_{sc}(\lambda)\{1+R_{_{M,\gamma}}(\lambda)\} \tag{25}$$

$$R_{_{M,\gamma}}(\lambda) = \gamma^{M+2}\frac{C_{M+2}}{(M+2)!}\frac{1}{g_{sc}(\lambda)}\frac{d^{M+2}g_{sc}(\lambda)}{d\lambda^{M+2}}$$

$$C_{M+2} = (-1)^{M/2}\frac{1.3.5.....(M+1)}{2^{(M+2)/2}}, \quad M \text{ even},$$

$$with \quad \lambda-\epsilon_0 \gg \gamma \gtrsim \overline{\hbar\omega}$$

Eq.(25) is fundamental and gives the straightforward link between the semiclassical level density $g_{sc}(\lambda)$, and the Strutinsky level density $\overline{g}_{_{M,\gamma}}(\lambda)$ in the asymptotic limit $\lambda-\epsilon_0 \gg \gamma$, with the necessary condition of the smoothing procedure $\gamma \gtrsim \overline{\hbar\omega}$.

It should be noted that it is $\overline{g}_{_{M,\gamma}}(\lambda)$ which is deduced from $g_{sc}(\lambda)$ and not the opposite. Moreover, $g_{sc}(\lambda)$ does not depend on any free parameter. Therefore $g_{sc}(\lambda)$ must be considered as the "true" smooth level density (the so-called smooth component of the quantum density (2)), and λ is its Fermi level.

The quantity $R_{_{M,\gamma}}(\lambda)$ is the remainder of the averaging. From (25), it can easily be identified with the relative error:

$$|R_{_{M,\gamma}}(\lambda)| \approx \left|\frac{g_{sc}(\lambda)-\overline{g}_{_{M,\gamma}}(\lambda)}{g_{sc}(\lambda)}\right|$$

and represents the noise (for the density of states) of the Strutinsky method. In actual calculations, it is implicit, and thus unknown. It is contained intrinsically in $\overline{g}_{_{M,\gamma}}(\lambda)$.

It is easy to check from (25) that the coefficient $C_{M+2}/(M+2)!$ in the remainder decreases theoretically to zero as M increases to infinity (λ,γ being fixed), provided that $g_{sc}(\lambda)$ is sufficiently regular. This in principle

improves the average. Nevertheless, we have seen in subsec.II E that large values of M involve necessary a slight increasing of γ in the smoothing procedure, which in turn increases somewhat the remainder as it can easily be seen from (25). Thus, it is not possible to reduce the remainder without ending.

In practical cases, the "optimal choice" $M \sim 16-30$ leads to a very good precision, i.e. $|R_{M,\gamma}(\lambda)| < 0.01$.

From Rel.(25) it is clear that the dependency on the two parameter (M,γ) becomes more and more weak as the remainder decreases to zero.

The only one special case where the remainder vanishes rigorously is that one where $g_{sc}(\lambda)$ is a pure polynomial of degree less or equal to M. This happens in the harmonic oscillator case. For this reason, the Strutinsky method must not be "judged" in this example when $M \geqq 2$.

Fundamentally, the Strutinsky level density appears in (25) only as an approximation (and thus is not strictly equivalent as it is often claimed) to the semiclassical level density. Consequently, the smooth Strutinsky energy Eq.(9), and the Strutinsky shell correction of Eq.(11) must also be considered as an approximations to the respective semiclassical quantities given by Eq.(20) and Eq.(22).

In fact, we shall see in the next subsection that the remainder tends also to zero with λ like $(\gamma/\lambda)^{M+2}$, and thus becomes negligible only in the "asymptotic limit" $(\gamma/\lambda) \ll 1$.

B. The relative error on the Strutinsky level density in two special cases

It is instructive, to apply our result (25) for the cases seen previously, i.e., the harmonic oscillator (16) and the cubic box (18) with the previous assumptions $\lambda - \epsilon_0 \gg \gamma \gtrsim \overline{\hbar\omega}$. For these calculations we choose $M = 0$ and $M = 2$ (M must be even).

For the harmonic oscillator case, using $g_{sc}(\lambda)$ from Eq.(16), we find:

For $M = 0$

$$\overline{g}_{M=0,\gamma}(\lambda) \approx g_{sc}(\lambda)\left[1 + \frac{1}{2}\frac{\gamma^2}{\lambda^2}\right], \quad with \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega} \tag{26}$$

(Here of course, the mean spacing between the shells is constant, and we have simply $\overline{\hbar\omega} = \hbar\omega$).

For $M = 2$

$$\overline{g}_{M=2,\gamma}(\lambda) \approx g_{sc}(\lambda)\left[1 + 0\right], \quad with \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega} \tag{27}$$

Since the semiclassical level density is a parabola, the derivative which appears in the remainder $R_{M,\gamma}$ in Eq.(25) cancels for $M \geq 2$, therefore one obtains the exact result (the remainder is 0). One should not be too "impressed" by this case (see subsection IV A).

For the infinite cubic box , using $g_{sc}(\lambda)$ from Eq.(18) we get for $M = 0$ and $M = 2$:

$$\overline{g}_{M=0,\gamma}(\lambda) \approx g_{sc}(\lambda)\left[1 - \frac{1}{16}\frac{\gamma^2}{\lambda^2}\right], \quad with \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega} \tag{28}$$

$$\overline{g}_{M=2,\gamma}(\lambda) \approx g_{sc}(\lambda)\left[1 + \frac{15}{512}\frac{\gamma^4}{\lambda^4}\right], \quad with \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega} \tag{29}$$

There also, for both cases, we obtain very similar relations.

Thus, in these four cases, the Strutinsky level density approaches the semiclassical level density, and the relative error (remainder) tends to zero only in the asymptotic limit $\gamma/\lambda \ll 1$. Moreover it is clear that in this limit, the Strutinsky densities becomes practically independent on the smoothing parameters (γ, M).

In realistic cases, the Fermi level λ is fixed for a given nucleus. It turns out that for medium and heavy nuclei, the quantity λ lies several units of $\overline{\hbar\omega}$ above the bottom of the well , since $\overline{\hbar\omega} \approx \gamma$, the quotient γ/λ is thus small and the remainder is practically negligible. Consequently, for these cases, the Strutinsky density of states is very close to the semiclassical level density.

The relative error of the Strutinsky density for the cubic box is illustrated in Fig. 2.

In Fig.2a we compare the "numerical" Strutinsky level density (curve a) calculated by means of Eq.(5) to the semiclassical density (curve b) given by Eq.(18). Apart from the region near zero (very small λ), and in spite of the "low" order $M = 0$ of the curvature correction, It is clear, that the two densities are practically indistinguishable. The theoretical link between both densities is given by Eq.(28)

In Fig.2b, we can see that the "numerical" relative error $(g_{sc} - \overline{g}_{M=0,\gamma})/g_{sc}$ of the Strutinsky density (denoted by (b-a)/b) with respect to the semiclassical density (regarded as the true smooth density), is very small, especially in the asymptotic limit ($(\gamma/\lambda) \ll 1$). In the latter, this error becomes close to the theoretical value $\gamma^2/16\lambda^2$ given by Eq.(28).

C. The relative error on the Strutinsky energy in the two previous cases

The average energy $\overline{E}_{M,\,\gamma}(\lambda)$ can be deduced by combining Eq.(9) and Eq.(25) with the assumptions of the asymptotic limit and the necessary condition of smoothing made in Eq.(25):

$$\overline{E}_{M,\,\gamma}(\lambda) \approx E_{sc}\,(\lambda)\left[1+\rho_{_{M},\gamma}\,(\lambda)\right] \tag{30}$$

$$\rho_{_{M},\gamma}\,(\lambda) = \frac{S_{_{M},\gamma}\,(\lambda)}{E_{sc}(\lambda)} \tag{31}$$

$$S_{_{M},\gamma}\,(\lambda) = \frac{\gamma^{M+2}C_{M+2}}{(M+2)!}\int\limits_{-\infty}^{\lambda}\epsilon\frac{d^{M+2}g_{sc}(\epsilon)}{d\epsilon^{M+2}}d\epsilon \tag{32}$$

$$with \quad \lambda-\epsilon_0 \gg \gamma \gtrsim \overline{\hbar\omega} \tag{33}$$

where $\rho_{_{M},\gamma}\,(\lambda)$ and $S_{_{M},\gamma}\,(\lambda)$ are respectively the relative and the absolute errors on the smooth (Strutinsky) energy $\overline{E}_{M,\,\gamma}(\lambda)$.

We know from Eq.(25) that $\overline{E}_{M,\,\gamma}(\lambda)$ must be considered as an approximation to $E_{sc}(\lambda)$. Besides, unlike $\overline{E}_{M,\,\gamma}(\lambda)$, the quantity $E_{sc}(\lambda)$ does not depend on any unphysical parameter. As before the remainder $\rho_{_{M},\gamma}\,(\lambda)$ of the Strutinsky energy must be related to the relative error:

$$\left|\rho_{_{M},\gamma}\,(\lambda)\right| \approx \left|\frac{E_{sc}\,(\lambda)-\overline{E}_{M,\,\gamma}(\lambda)}{E_{sc}\,(\lambda)}\right| \tag{34}$$

Once again, in order to illustrate some features of the Strutinsky method we apply the above result for the harmonic oscillator and for the cubic box with $M=0$ and $M=2$.

For the harmonic oscillator:

$$\overline{E}_{M=0,\,\gamma}(\lambda) \approx E_{sc}(\lambda)\left[1+\frac{\gamma^2}{\lambda^2}\right], \quad with \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega} \tag{35}$$

$$\overline{E}_{M=2,\,\gamma}(\lambda) \approx E_{sc}(\lambda)\left[1+0\right], \quad with \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega} \tag{36}$$

Where $E_{sc}(\lambda)$ of the harmonic oscillator is given in appendix B.

In the same way, we obtain for the cubic box:

$$\overline{E}_{M=0,\,\gamma}(\lambda) \approx E_{sc}(\lambda)\left[1-\frac{5}{16}\frac{\gamma^2}{\lambda^2}\right], \quad with \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega} \tag{37}$$

$$\overline{E}_{M=2,\,\gamma}(\lambda) \approx E_{sc}(\lambda)\left[1-\frac{25}{512}\frac{\gamma^4}{\lambda^4}\right], \quad with \quad \lambda \gg \gamma \gtrsim \overline{\hbar\omega} \tag{38}$$

Where $E_{sc}(\lambda)$ of the cubic box is also given in appendix B.

Thus, in the asymptotic limit $(\gamma/\lambda) \ll 1$ (i.e. for medium and heavy nuclei), as for the density of states (25), the relative error is small, and we have also $\overline{E}_{M,\,\gamma}(\lambda) \approx E_{sc}(\lambda)$. Thus, for the smooth energy, the Strutinsky method is a good approximation of the semiclassical method. A straightforward consequence is that the smooth (Strutinsky) energy $\overline{E}_{M,\,\gamma}$ becomes practically independent on the smoothing parameters (M,γ) in this limit.

We give in Fig. 3 an illustration of the relative error for the Strutinsky energy for the cubic box

Fig.3a: Same conclusions as Fig.2a, i.e. $\overline{E}_{M=0,\,\gamma}(\lambda)$ and $E_{sc}(\lambda)$ are indistinguishable

Fig.3b: There also, the relative error on the Strutinsky energy (with respect to the semiclassical energy) tends toward zero in the asymptotic limit $(\gamma/\lambda) \ll 1$ and approaches the theoretical value $5\gamma^2/16\lambda^2$ given by Eq.(37).

D. The new understanding of the plateau condition on the average (Strutinsky) energy

As seen before, the relative error plays a major role in the Strutinsky energy.

From Rel.(34), it is clear that if $\left|\rho_{_{M},\gamma}\,(\lambda)\right| \ll 1$, the relative variations of the Strutinsky energy $\overline{E}_{M,\,\gamma}(\lambda)$ *are small compared to* $\overline{E}_{M,\,\gamma}(\lambda)$ itself (or to $E_{sc}(\lambda)$).

For instance, if one plots $\overline{E}_{M,\,\gamma}(\lambda)$ as a function of the parameter γ (M and λ being constant) it appears a "plateau" in the graph. This means that $\overline{E}_{M,\,\gamma}(\lambda)$ is "practically constant at the scale of its own value" (at least in the interval $\lambda \gg \gamma \gtrsim \overline{\hbar\omega}$), i.e.:

$$\left(\frac{\Delta\overline{E}_{M,\,\gamma}(\lambda)}{\overline{E}_{M,\,\gamma}(\lambda)}\right)_{\lambda\gg\gamma\gtrsim\overline{\hbar\omega}} \ll 1 \tag{39}$$

(which is close to (34)). This does not necessarily mean that the derivative of $\overline{E}_{M,\,\gamma}(\lambda)$ cancels as in the traditional plateau condition [18]. The same remark holds for the Strutinsky density.

We must point out that the relative error is proportional to the quantity $(\gamma/\lambda)^{M+2}$, so that the plateau is improved at large values of M.

Fig. 4 shows an illustration of the plateau (defined by (39)) for the energy in the cubic box case

Fig.4a: The Strutinsky energy $\overline{E}_{M,\,\gamma}$ of the cubic box is plotted as function of γ for four values of the order M. The particle-number is fixed arbitrarily at $N_0=200$ with a Fermi level $\lambda = 64.255E_0$. It is clear that the fluctuations $\Delta\overline{E}_{M,\,\gamma}$ are small compared to $\overline{E}_{M,\,\gamma}$. At this "scale" a clear plateau is noticed.

Fig.4-b: The same figure as Fig.4-a at a "reduced scale" shows the important variations of the plateau, especially on the r.h.s of the figure. If we continue to "zoom in" the curve, it appears several minima and maxima (i.e. $\partial\overline{E}_{M,\,\gamma}/\partial\gamma = 0$). Some of them, have nothing to do with a plateau. For example, in the vicinity of $\gamma \approx 154\ E_0$ a minimum occurs for the order $M=16$ which does not really belong to any plateau. Thus our "macroscopic" definition of the plateau seems more "adapted" than the old version based on the "stationarity" of $\overline{E}_{M,\,\gamma}$ with respect to γ. In fact, it contains implicitly the concept of

the relative error which plays a central role in the numerical applications in the method. Indeed the minimization of the relative error (see below) avoids the ambiguity of the (old) plateau condition, because a stationary point is not necessary a plateau, whereas the minimization of the relative error leads indisputably to the true value (at the very least to the optimal value) of the smooth energy, an thence of the shell correction (see below).

E. The Strutinsky shell correction

1. The critical point of the Strutinsky method

First, one must recall that the Strutinsky shell correction and the semiclassical shell correction are respectively defined through Rel.(11) and (22), i.e.

$\delta\overline{E}_{M,\gamma} = \sum_{occupied} \epsilon_n - \overline{E}_{M,\gamma}(\lambda)$,

$\delta E_{sc} = \sum_{occupied} \epsilon_n - E_{sc}(\lambda)$

Subtracting the second equation from the first, and using Rel.(30), one obtains a straightforward relation between these two quantities.:

$$\delta\overline{E}_{M,\,\gamma}(\lambda) \approx \delta E_{sc}(\lambda) - S_{M,\gamma}(\lambda) \tag{40}$$

Since $\overline{E}_{M,\gamma}(\lambda)$ is considered as an approximation to $E_{sc}(\lambda)$ (see previous subsection), the Strutinsky shell correction $\delta\overline{E}_{M,\,\gamma}(\lambda)$ must be also regarded as an approximation to the semiclassical shell correction $\delta E_{sc}(\lambda)$. In this respect, $S_{M,\gamma}(\lambda)$ represents the same absolute error in both formulae (30,40). However, the essential point is that, this error has not the same importance in these two results

Indeed, the two shell corrections $\delta E_{M,\,\gamma}(\lambda)$, and $\delta E_{sc}(\lambda)$ are obtained as the difference between two close large numbers (i.e. the sum of single-particle energies and their averages) therefore they are significantly smaller compared to these quantities (i.e. $\overline{E}_{M,\,\gamma}$ or E_{sc}).

For example, the Ref [12] gives for the case of ^{154}Sn (neutrons) the typical "realistic" values $\sum \epsilon_i = -1122.5\ MeV$, $\overline{E}_{M,\,\gamma} = -1132.0\ MeV$ (the order M is not précised in that work), and hence, the shell correction $\delta\overline{E}_{M,\,\gamma} = 9.5\ MeV$ is thus, much smaller than $\overline{E}_{M,\,\gamma}$. Consequently, the same absolute error $S_{M,\gamma}(\lambda)$ which is relatively small in Eq.(30) might become non negligible in Eq.(40) for the Strutinsky shell correction.

In addition, in a number of cases the shell correction might also become so small that the relative error (*in the shell correction*) has no longer a sense. Thus, for the shell correction, the relative error does not play the same leading role as for the Strutinsky energy (or the Strutinsky density), so that the (Strutinsky) shell correction might become strongly dependent to the choice of the parameter γ. This means that the error could exceed the shell correction itself if this error is not optimized (i.e. minimized).

2. The optimization of the method with the "rule of the relative remainder R.R.R".

The shell correction is defined as the difference between two quantities $\sum \epsilon_i$, and $\overline{E}_{M,\,\gamma}(\lambda)$. Only the latter depends on the parameter γ (and also M) through the remainder $\rho_{M,\gamma}(\lambda)$ from (30). By minimizing this remainder (i.e. the relative error) with respect to γ, we make $\overline{E}_{M,\,\gamma}(\lambda)$ as close as possible to E_{sc}, therefore we make $\delta\overline{E}_{M,\,\gamma}(\lambda)$ as close as possible to $\delta E_{sc}(\lambda)$ (i.e. the true shell correction). Thus, the minimization of the relative error made on $\overline{E}_{M,\,\gamma}(\lambda)$, should lead to the independency (or at least to a weak dependence) of $\delta\overline{E}_{M,\,\gamma}(\lambda)$ on the parameters (γ, M). Thence, we can affirm that it is the minimization of this relative error which is the source of the plateau, not the opposite. This should be the most appropriate way for finding the true (or the best) value of the shell correction. Fig.5 displays a practical illustration of this minimization (the so-called "rule of relative remainder").

We show in Fig.5a how to find the optimal value for the parameter γ in the cubic box case. We again consider in Fig.5a the case given in Fig.4a

The steps are the following:

- First we calculate the Strutinsky energy at the Fermi level $\overline{E}_{M,\,\gamma}(\lambda)$ as a function of the parameter γ (λ being fixed), for some close values of the order M.
- We must minimize the remainder of Rel.(34) as follows:

$$\left|\frac{\partial}{\partial\gamma}\rho_{M,\gamma}(\lambda)\right| = \left|\frac{\partial}{\partial\gamma}\frac{E_{sc}(\lambda) - \overline{E}_{M,\,\gamma}(\lambda)}{E_{sc}(\lambda)}\right| \approx 0$$

$$= \left|\frac{\frac{\partial\overline{E}_{M,\,\gamma}(\lambda)}{\partial\gamma}}{E_{sc}(\lambda)}\right| \approx \left|\frac{\frac{\partial\overline{E}_{M,\,\gamma}(\lambda)}{\partial\gamma}}{\overline{E}_{M,\,\gamma}(\lambda)}\right|$$

- Then, this quantity is plotted as a function of γ for each value of M. Thence, we should look for the minimum of this function (relative error).

However for a fixed M, this function has an oscillatory behavior (around zero) which leads to several local minima. Nevertheless, due to the fact that these curves do not cancel simultaneously, it is possible to remove these unpleasant oscillations by considering the mean relative error over some (relative close) values of M.

The mean relative error (over $M = 16, 20, 24, 28$) on the Strutinsky energy is plotted against γ. The minimum (optimal) value is found to be about $\gamma_{opt} \approx 28.6E_0$ and corresponds effectively to the best value (see Fig.5b)

In Fig.5b, we note a good agreement between the true value (semiclassical) given by the upper straight line $\overline{E}_{sc} \approx 8093.97E_0$ and the Strutinsky values.

In fact, for the optimized γ, the calculated values are $\overline{E}_{16,\,\gamma_{opt}} \approx 8094.52E_0$, $\overline{E}_{20,\,\gamma_{opt}} \approx 8094.64E_0$, $\overline{E}_{24,\,\gamma_{opt}} \approx 8095.21E_0$, $\overline{E}_{28,\,\gamma_{opt}} \approx 8096.31E_0$, for $M = 16, 20, 24, 28$.
At last the sum of single-particle energies is $\sum_{occ.states} \epsilon_i \approx 7842E_0$.

The true shell correction $\delta\overline{E}_{sc} \approx -251.97E_0$, and the corresponding Strutinsky shell corrections are thus: $\delta\overline{E}_{16,\,\gamma_{opt}} \approx 252.52E_0$, $\delta\overline{E}_{20,\,\gamma_{opt}} \approx 252.64E_0$, $\delta\overline{E}_{24,\,\gamma_{opt}} \approx 253.21E_0$, $\delta\overline{E}_{28,\,\gamma_{opt}} \approx 254.31E_0$, which are in good agreement with the true (exact) value. Without optimization the results of the Strutinsky shell correction will certainly be random.

F. Case of realistic wells:

1. The Strutinsky level density

First, we must note that the spectrum of the finite potential is composed of discrete negative levels plus a continuum. For this potential, the definition of the exact level density (2) must be modified by adding an appropriate continuous expression $g_c(\epsilon)$:

$$g_o(\epsilon) = \sum_n \delta(\epsilon - \epsilon_n) + g_c(\epsilon) \tag{41}$$

For spherical potentials, the continuum is defined by the scattering phase shift, whereas for the deformed case it can be solved by the more complicated S-matrix method (see [8]).

Next, one recalls that the result (25) (which is the basis of the present work) comes from Eq.(6). The latter is valid for any smooth potential regardless whether it is infinite or not. Indeed, it is to be noted that the interval of averaging in (6) goes from $-\infty$ up to $+\infty$ so that the preceding demonstration remains still valid for a finite well. One has simply to add the continuum of (41) to the discrete spectrum into this integral. Thence, as for infinite potentials, it is clear that the Strutinsky's level density should also be an approximation to the semiclassical level density for finite wells.

In practice, the rigorous treatment of the continuum is not easy. The standard recipe consists of using the discrete positive energies to "simulate" this continuum [9]. These energies are usually obtained by diagonalizing the Hamiltonian matrix in a truncated harmonic oscillator basis. In fact, this delicate problem seems now to be solved by the so-called GFOE method (Green's function oscillator expansion) [12] which improves the standard method..

2. The semiclassical level density

It is well-known that the level density of finite potential becomes singular at the top of the well [24],[8]. For this reason, it is not possible to find a local polynomial approximation to the semiclassical level density in the vicinity of this singularity. In other words, the least square averaging (3) does not hold in this case, precisely because $g_{sc}(\lambda) \to \infty$, as $\lambda \to 0$, i.e. at the zero-energy. This explains why the two methods do not lead to the same results, especially for the weakly bound nuclei. Far from the zero-energy there is no problem.

3. Comparison between the two level densities

It would be interesting to determine the limit where the Strutinsky level density deviates significantly from the semiclassical density. To this end, we will be comparing numerically the Strutinsky level density to the semiclassical (Wigner-Kirkwood) level density by employing the result of Ref [23]:

$$g_{sc}(\lambda) = \frac{dN_{sc}(\lambda)}{d\lambda_{sc}} \tag{42}$$

with:

$$N_{sc} = \frac{1}{3\pi^2}\left(\frac{2m}{\hbar^2}\right)^{3/2} \int_0^{r_{sc}} d^3r \left[(\lambda_{sc} - U)^{3/2} + \left(\frac{2m}{\hbar^2}\right)^{-1} \Omega\right] \tag{43}$$

$$\Omega = \left[\frac{3}{4}\kappa^2 \left(\vec{\nabla} f_{so}\right)^2 (\lambda_{sc} - U)^{1/2} - \frac{1}{16}\nabla^2 U (\lambda_{sc} - U)^{-1/2}\right]$$

This formula contains the "classical" Thomas-Fermi term plus an $\hbar^2$ Wigner-Kirkwood correction. In this formula $U(\vec{r})$ is the central mean potential which contains also the Coulomb interaction for the protons, and $f_{so}(\vec{r})$ is the spin-orbit interaction. The classical turning points r_{sc} are defined by $U(\vec{r_{sc}}) = \lambda_{sc}$ where λ_{sc} is the Fermi level
The numerical integration giving N_{sc} is made with the help of an "improved" Gauss-Legendre quadrature formula.
The eigenvalues used in the Strutinsky level density are calculated by the code published in [26].
In the two methods we employ strictly the same Hamiltonian and the same set of parameters, i.e. we use the Woods-Saxon potential with spin-orbit term and the Coulomb potential for the protons. For this test we work with the ^{208}Pb (neutrons) with a spherical nuclear shape. The parameters (in MeV, fm) are: $V_0 = -47.083MeV$, $a_v = 0.66MeV$, $R_V = 7.36fm$, $\varkappa = 12.0MeVfm^2$, $a_{so} = 0.55fm$, $R_{so} = 6.698fm$. Their definition is given in [26].

Thus, in Fig.6, we have drawn the semiclassical level density (denoted by semicl.) and the Strutinsky density as function of the Fermi level for three cases (the numerical values of the smoothing parameters are given in the figure).

- We can check in the three cases that the Strutinsky level density is practically equal to semiclassical density in the "intermediate" region (between the top and the bottom of the well) irrespectively of the order M of the smoothing procedure. Indeed, we have shown in the subsection IV B that in the asymptotic limit (i.e. for medium and heavy nuclei) the Strutinsky density of states (not the Strutinsky shell correction !) should not be very sensitive to both free parameters of the method. However, although with $M = 0$ one obtains a good relative error on the density of states, one improves more this error at sufficient large values of M.

- As expected, due the reason invoked above, Fig.6 shows that the Strutinsky densities differ from the semiclassical result essentially at the top of the well. In the "intermediate region" there is no difference. Near the singularity, it is more advantageous to choose high values for the order M . With $M = 30$, the Strutinsky calculation seem to work reasonably well up to about $-2.5\ MeV$, beyond this limit the precision is lost.

- However, we should not forget that it is the semiclassical density which is the "true" quantity. Due to the importance of the difference between the two methods near the zero-energy, the semiclassical method must in principle be preferred for the weakly bound nuclei.

V. CONCLUSION:

Although this paper explains a number of aspects and "subtleties" of the Strutinsky method, we will insist on some essential points:

1) The Strutinsky level density appears in the fundamental Rel.(25) only as an approximation (and is not strictly equivalent as it is often claimed) to the semiclassical level density. Consequently, the shell correction calculated by the Strutinsky's method should also be considered as an approximation to the semiclassical shell correction.

2) Semiclassical quantities such as the level density, the energy, the shell correction must be considered as the "true" quantities compared to those obtained with the Strutinsky method. Moreover, they do not depend on any free parameter.

Unlike the semiclassical method, the Strutinsky method contains an intrinsic noise (remainder). The ambiguity of the method comes from the dependence on the two free parameters through this remainder.

3) It turns out that the remainder is proportional to $(\gamma/\lambda)^M$ and is defined in this paper as the relative error. In the asymptotic limit $(\gamma/\lambda) \ll 1$, i.e. for medium and heavy nuclei, the relative error is small, especially for higher M. Therefore, it is found that the Strutinsky method gives good results for the average level density, and the average energy. In these cases the dependency on the free parameters is weak.

On the contrary, in the shell correction the relative error is no longer small. The shell correction might become strongly (γ, M)-dependent. The choice of these two free parameters must be treated with care. In this context, in order to minimize the relative error, we propose the "rule of the relative remainder (RRR)".

4) For realistic potentials, the semiclassical level density admits a singularity at the top of the well. Since the Strutinsky method is a least-squares approximation to the semiclassical level density (demonstrated in this paper), the averaging fails near this singularity. In this case, the two densities are different, and it is not surprising to note a strong dependence on the parameters $(\gamma; M)$ in this region, even if the continuum is treated properly. Consequently, for the weakly bound nuclei (drip-line) it is better to use the semiclassical method.

Our personal conclusion, is that the semiclassical method with a "good numerical treatment" should, in theory, be quite superior to the Strutinsky method. The latter can be considered only as a good palliative method.

APPENDIX A: CALCULATION OF THE INTEGRAL $I(M)$

$$I(M) = \int_{-\infty}^{\infty} x^{M+2} \widetilde{P_M}(x) \exp(-x^2) dx, \qquad \text{(see subsec.IV A)}$$

First, one must note that $\widetilde{P_M}(x)$ of (5) can be expressed as $\widetilde{P_M}(x) = \dfrac{H_M(0)}{2^{M+1} M! \sqrt{\pi}} \dfrac{H_{M+1}(x)}{x}$.

Indeed, with the help of the Christoffel-Darboux formula (chap 22 of [17]):

$$\sum_{k=0}^{n} \frac{H_k(x) H_k(y)}{2^k k!} = \frac{H_{n+1}(x) H_n(y) - H_{n+1}(y) H_n(x)}{2^{n+1} n! (x-y)}$$

one finds for our case:

$$\widetilde{P}_M(x) = \sum_{m=0}^{M} \frac{H_m(0)}{m! 2^m \sqrt{\pi}} H_m(x)$$

$$= \frac{H_{M+1}(x) H_M(0) - H_{M+1}(0) H_M(x)}{2^{M+1} M! \sqrt{\pi} (x-0)},$$

Since M is even, $H_{M+1}(0) = 0$, this gives the cited expression

To calculate the integral $I(M)$, we have to replace $\widetilde{P_M}(x)$ by the preceding result. We obtain:

$$I(M) = \frac{H_M(0)}{2^{M+1} M! \sqrt{\pi}} \int_{-\infty}^{\infty} x^{M+1} H_{M+1}(x) \exp(-x^2) dx$$

Now we use the following property [17]:

$$\int_{-\infty}^{\infty} t^k H_k(st)\exp(-t^2)dt = \sqrt{\pi}k!P_k(s)$$

where $P_k(s)$ is a Legendre polynomial. For our purpose, we choose $s=1$, with $P_k(1)=1$. Making $k=M+1$ in the above result, one finds:

$$\int_{-\infty}^{\infty} x^{M+1}H_{M+1}(x)\exp(-x^2)dx = \sqrt{\pi}(M+1)!$$

so that:

$$I(M) = \frac{H_M(0)}{2^{M+1}M!\sqrt{\pi}}\sqrt{\pi}(M+1)! = \frac{H_M(0)}{2^{M+1}}(M+1)$$

Where $H_M(0)$ is given in the subsect.II D. Finally, the result can be cast under the following form:

$$I(M) = \frac{(-1)^{M/2}}{2^{(M+2)/2}}1.3.5.....(M+1)$$

APPENDIX B: TWO APPLICATIONS OF THE EULER MACLAURIN FORMULA (EML)

In the present work, to obtain some analytical results we employ the Euler-MacLaurin formula (EML) [17].

$$\sum_{k=1}^{n-1}F(k) = \int_0^n F(k)dk - \tfrac{1}{2}[F(0)-F(n)]$$
$$+\tfrac{1}{12}[F'(n)-F'(0)] - \tfrac{1}{720}[F'''(n)-F'''(0)] + ...$$

Of course this formula can be used to calculate discrete finite sums. But here, the interest of this formula is its application to the determination of the asymptotic behavior ($n\to\infty$) of the discrete sum. In explicit terms, if we take a few terms (integral plus a few derivatives) in this formula, we obtain a quantity which is equivalent to the discrete sum. This means that the error (difference between the discrete sum and its equivalent from the EML formula) tends to zero as n increases to infinity.

In general, the higher orders of this formula are divergent and must be simply ignored. For this reason, an asymptotic expansion does not exceed three or four terms.

We apply this formula for two cases:

- The harmonic oscillator where we take just the integral in the EML formula, neglecting thus the divergent terms (Dirac delta functions) in the result:

$$\sum_{n=0}^{\infty} D(n)\ \delta(\epsilon-(n+3/2)\hbar\omega)$$
$$\approx \frac{1}{\hbar\omega}\int_0^{\infty} D(n)\ \delta\left[\frac{\epsilon}{\hbar\omega}-(n+3/2)\right]dn = g_{sc}(\epsilon)$$

$D(n)=(n+1)(n+2)/2$ is the degeneracy of the level n, we find:

$$g_{sc}(\epsilon) \approx \frac{1}{2\hbar\omega}\left[\left(\frac{\epsilon}{\hbar\omega}\right)^2 - \frac{1}{4}\right]$$

Now, it is easy to deduce the semiclassical energy:

$$\overline{E}_{sc}(\lambda) \approx \int_0^{\lambda}\epsilon\overline{g}_{sc}(\epsilon)d\epsilon = \frac{\lambda^4}{8(\hbar\omega)^3} - \frac{\lambda^2}{16\hbar\omega}$$

- In the cubic box the degeneracy is unknown, and we have to evaluate a threefold integral. We work with a "basic" EML formula, i.e without derivatives:

$$\sum_{k=1}^{\infty}F(k) \approx \int_0^{\infty}F(k)dk - \tfrac{1}{2}F(0)$$

Starting from that, we apply this formula in the case of the threefold sum:

While all axes are equivalent, we obtain

$$\sum_{n_x=0}^{\infty}\sum_{n_y=0}^{\infty}\sum_{n_z=0}^{\infty}F(n_x,n_y,n_z) =$$
$$\int_0^{+\infty}\int_0^{+\infty}\int_0^{+\infty}F(n_x,n_y,n_z)dn_xdn_ydn_z$$
$$-(3/2)\int_0^{+\infty}\int_0^{+\infty}F(n_x,n_y,0)dn_xdn_y$$
$$+(3/4)\int_0^{+\infty}F(n_x,0,0)dn_x - (1/8)F(0,0,0)$$
$$= I_3+I_2+I_1+I_0 \quad \text{(respectively)}$$

Here $F(n_x,n_y,n_z)=\delta\left(\epsilon-(n_x^2+n_x^2+n_x^2)E_0\right)$.

Using the spherical coordinates we find

$$I_3 = \frac{\pi}{4}\frac{\sqrt{\epsilon}}{E_0^{3/2}},\qquad I_2 = -\frac{3\pi}{8E_0},\qquad I_1 = \frac{3}{8E_0^{1/2}\sqrt{\epsilon}},$$
$$I_0 = -\frac{1}{8}\delta(\epsilon)$$

Here also we omit I_0(delta function)

$$g_{sc}(\epsilon) = \frac{\pi}{4}\frac{\sqrt{\epsilon}}{E_0^{3/2}} - \frac{3\pi}{8E_0} + \frac{3}{8E_0^{1/2}\sqrt{\epsilon}}$$

Therefore:

$$\overline{E}_{sc}(\lambda) \approx \int_0^{\lambda}\epsilon\overline{g}_{sc}(\epsilon)d\epsilon = \frac{\pi}{10}\frac{1}{E_0^{3/2}}\lambda^{5/2} - \frac{3\pi}{16E_0}\lambda^2 + \frac{1}{4E_0^{1/2}}\lambda^{3/2}$$

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